Adiabatic approximation with exponential accuracy for many-body systems and quantum computation

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We derive a version of the adiabatic theorem that is especially suited for applications in adiabatic quantum computation, where it is reasonable to assume that the adiabatic interpolation between the initial and final Hamiltonians is controllable. Assuming that the Hamiltonian is analytic in a finite strip around the real time axis, that some number of its time-derivatives vanish at the initial and final times, and that the target adiabatic eigenstate is non-degenerate and separated by a gap from the rest of the spectrum, we show that one can obtain an error between the final adiabatic eigenstate and the actual time-evolved state which is exponentially small in the evolution time, where this time itself scales as the square of the norm of the time-derivative of the Hamiltonian, divided by the cube of the minimal gap.

I. INTRODUCTION

The adiabatic approximation, with its long history [1, 2], has played a central role in quantum mechanics. This approximation states, roughly, that for a system initially prepared in an eigenstate (e.g., the ground state) $|\Phi_0(0)\rangle$ of a sufficiently slowly varying Hamiltonian $h(t)$, the time evolution governed by the Schrödinger equation $i\frac{\partial|\psi(t)\rangle}{\partial t} = h(t)|\psi(t)\rangle$ will approximately keep the actual state $|\psi(t)\rangle$ of the system in the corresponding instantaneous ground state $|\Phi_0(t)\rangle$ of $h(t)$, provided that there are no level crossings. Quantitative statements of this approximation have a long history, with rigorous results appearing only in recent years. Let $|\Phi_j(t)\rangle$ ($j \in \{0, 1, 2, \ldots\}$) denote the instantaneous eigenstate of $h(t)$ with energy $e_j(t)$, i.e., $h(t)|\Phi_j(t)\rangle = e_j(t)|\Phi_j(t)\rangle$. The simplest and one of the oldest traditional versions of the adiabatic approximation states that the Hamiltonian must be slow with respect to the time scale dictated by the ratio of a matrix element of the time-derivative of the Hamiltonian to the square of the spectral gap $d \equiv \min_{0\le t\le T; j>0}[e_j(t) - e_0(t)]$ [3]. Namely, the fidelity between the actual final state and the adiabatic eigenstate satisfies $|\langle\psi(T)|\Phi_0(T)\rangle|^2 \ge 1 - \varepsilon^2$, where $\varepsilon \equiv \max_{0\le t\le T; j>0}[|\langle\Phi_j(t)|\dot{h}(t)|\Phi_0(t)\rangle|/d^2]$. Unfortunately this simple criterion — while often useful, and widely used (e.g., in Refs. [4–6]) — is in fact neither necessary nor sufficient in general, as recently confirmed experimentally [7]. The inadequacy of the traditional criterion is well known and the criterion has been replaced by rigorous general results as can be found, e.g., in Refs. [8–12], and in the presence of noise, in Ref. [13]. All these rigorous results are more severe in the gap condition than the traditional criterion, and they involve a power of the *norm* of time derivatives of the Hamiltonian, rather than a transition matrix element. In this work we revisit the adiabatic approximation and prove a version of the adiabatic theorem that is motivated by recent developments in the field of quantum information science [14], namely the idea of adiabatic quantum computation (AQC) [4, 5].

AQC offers a fascinating paradigm for exploiting quantum mechanics in order to obtain a speedup for classically difficult computational problems. In AQC one solves a computational problem by adiabatically modifying a Hamiltonian whose initial ground state $|\Phi_0(0)\rangle$ encodes the input and whose final ground state $|\Phi_0(T)\rangle$ encodes the output. The time T taken to reach the final ground state is the "running time" of the quantum adiabatic algorithm, which one would like to minimize while at the same time minimizing the distance δ between the actual final state $|\psi(T)\rangle$ and the desired final ground state $|\Phi_0(T)\rangle$. This, of course, is the subject of the quantum adiabatic theorem, and provides the motivation for the present paper. In quantum computation one is interested in how T scales with problem size, which is typically encoded into the system size needed to represent the problem, e.g., the number n of quantum bits ("qubits"). Thus one expects both T and δ to scale with n. Our goal is two-fold. First, to determine the scaling properties of T and δ with n. Second, to show that δ can be made exponentially small in T.

AQC was first proposed as an approach to solving optimization problems such as satisfiability of Boolean formulas, by encoding a cost function into the Hamiltonian [4, 5]. However, it was soon realized that AQC is not limited to optimization: from a computational complexity perspective AQC is equivalent in power to all other models for universal quantum computation [15–19]. Namely, AQC and the other models for universal quantum computation can simulate one another with at most polynomial resource overhead. One of the reasons AQC has generated much interest recently is that it has a rich connection to well studied problems in condensed matter physics. For example, because of the dependence of T on the minimal gap, the performance of quantum adiabatic algorithms is strongly influenced by the type of quantum phase transition the same system would undergo in the thermodynamic limit [20, 21], thus offering an interesting perspective on the connection between quantum information methods and problems in condensed matter physics. AQC also appears to offer advantages over classical simulated annealing in finding an approximate ground state energy of a complex system [22].

To date, most AQC studies have relied on the traditional version of the adiabatic approximation. The main question we wish to

address in this work is: what is the rigorous tradeoff between a small final error δ and the scaling of the final time T with system size n, or any other relevant parameter? The reason one expects a dependence on n is clear from the "traditional criterion": the gap d and $\dot{h}(t)$ both depend on n. It has been known for some years in the mathematical physics literature that exponential accuracy in the form $\delta \leq e^{-cT}$ (c is some constant) is possible [9, 11], but the cost in terms of physical resources such as system size n has thus far not been quantified in rigorous proofs of the adiabatic theorem, even those specifically aimed at AQC [12, 13]. However, in AQC an understanding of the scaling of the running time with respect to problem size is of paramount importance.

It is further important to stress that in AQC one deals with "designer Hamiltonians", which contain controllable parameters beyond what is typically assumed in developments of the adiabatic approximation or proofs of the adiabatic theorem. That is, one envisions any number of "control knobs" which allow one to realize the goal of transforming the initial to the final Hamiltonian. Here we prove a version of the adiabatic theorem which focuses on one such control knob: the number N of vanishing initial and final time derivatives of the Hamiltonian. Furthermore, we assume that the Hamiltonian satisfies certain analyticity properties. Our theorem states, roughly, that for such Hamiltonians, the deviation between the final state and the desired (non-degenerate) adiabatic eigenstate can be made exponentially small in N, with a running time that scales as as a polynomial in N times the square of the supremum of the norm of the time derivative of the Hamiltonian, divided by the cube of the minimal gap. Since the scaling of $\sup_t \|\dot{h}\|$ and of the gap d can be quantified in terms of the system size n for situations of interest in AQC (see Section V B), this provides an answer to the scaling question we posed above, and our result should be particularly useful for AQC applications. In proving this result we rely on the adiabatic exponential error estimate and asymptotic expansion due to Hagedorn and Joye [11].

The structure of this paper is the following. We begin by stating our notation, definitions, and technical assumptions in Section II, and conclude this section with a statement of our version of the adiabatic theorem, including some remarks. Before proving this theorem, we provide pertinent background in Section III, including a brief summary of key results from Ref. [11]. Section IV is devoted to the proof of the adiabatic theorem. We provide a discussion in Section V, including a comparison of our version of the adiabatic theorem to some of the results of Refs. [12, 23]. In the same section we also analyze the scaling of the running time and error with system size, give an explicit result (Corollary 10) for second order quantum phase transitions, find the minimum adiabatic time T by optimizing the adiabatic interpolation and give an application of our adiabatic theorem in the open system setting (Theorem 4). We conclude in Section VI with some remarks about future directions. The reader who is not interested in the (lengthy) details of the proof of our adiabatic theorem can safely skip from the end of Section II to the discussion in Section V.

II. ADIABATIC THEOREM WITH ARBITRARY ACCURACY

In this section we state our adiabatic theorem. But before doing so, we introduce the requisite notation, definitions, and assumptions.

A. Schrödinger equation in dimensionless units

Let us start with the time-dependent Schrödinger equation

$$i\frac{\partial \psi}{\partial t} = h(t)\psi(t), \tag{1}$$

where we work in units of $\hbar \equiv 1$. Define the dimensionless Hamiltonian H as

$$H \equiv h/J, \tag{2}$$

where J is an arbitrary energy unit relative to which we shall express all other dimensional quantities.[1] Let us fix the final time T and define the dimensionless rescaled time τ as

$$\tau \equiv t/T = \epsilon J t. \tag{3}$$

This expresses the fact that for any given T we can always choose J so that ϵ, defined via

$$\epsilon \equiv 1/(JT), \tag{4}$$

[1] Since J is arbitrary it will drop out at the end of the analysis, when we reintroduce dimensional units.

is a small number, which we need for the asymptotic expansion below. The Schrödinger equation in dimensionless units now reads

$$i\epsilon\frac{\partial\psi}{\partial\tau} = H(\tau)\psi(\tau). \tag{5}$$

From now on most of our calculations will be done in dimensionless units.

B. Assumptions concerning the Hamiltonian, target state, and initial state

We shall need three assumptions. The first sets the stage for the family of Hamiltonians we shall be concerned with in this work. A Hamiltonian is by definition a self-adjoint (i.e., Hermitian) operator for real-valued times τ, and we shall be concerned with analytic continuations of the Hamiltonian.

Assumption 1 *$\{H(\tau)\}_{\mathrm{Re}\tau\in[0,\infty)}$ is a one-parameter family of bounded Hamiltonians of an n-body system, with the separable Hilbert space $\mathcal{H}_n = \mathcal{H}^{\otimes n}$.* [2] *Let $\gamma > 0$ denote the distance to the pole or branch point of $\{H(\tau)\}$ that is nearest to the real τ-axis in the complex τ-plane. The family $\{H(\tau)\}_{\mathrm{Re}\tau\in[0,\infty)}$ admits an analytic continuation to an open set $S_\gamma \equiv \{\tau : |\tau| < \gamma\} \cup \{\tau : |\mathrm{Im}(\tau)| < \gamma, \mathrm{Re}(\tau) \in [0,1]\} \cup \{\tau : |\tau - 1| < \gamma\}$, as depicted in Fig. 1.*[3]

Example 1 *In linear interpolations of the type $H(\tau) = x_0(\tau)H_0 + x_1(\tau)H_1$ (with H_0 and H_1 constant Hamiltonians such that $H(0) = H_0$ and $H(1) = H_1$), often used in AQC, if x_0 and x_1 are real-analytic functions, we can usually perform an analytic continuation. The height γ is dictated by possible singularities that appear because of complexification of the functions x_0 and x_1. E.g., $x_0(\tau) = (1-\tau)/(1+\tau^2)$ and $x_1(\tau) = 2\tau/(1+\tau^2)$ (satisfying $x_0(0) = x_1(1) = 1$ and $x_0(1) = x_1(0) = 0$), are real-analytic functions of $\tau \in \mathbb{R}$, but have singularities at $\tau = \pm i$. In this case, analytical continuation is possible within S_γ as depicted in Fig. 1, with $0 < \gamma < 1$.*

We denote the spectrum of an operator A by $\sigma(A)$. While our analysis applies equally well to finite and infinite-dimensional but bounded systems ($\dim\mathcal{H} < \infty$ or $= \infty$, respectively), for most applications the Hamiltonians of interest to us are those that are usually considered in quantum information theory, such as spin lattices with exchange interactions, for which $\dim\mathcal{H} < \infty$ and $\sigma(H(\tau))$ is discrete. Whenever our analysis below can be simplified by this assumption, we will explicitly assume that the instantaneous eigensystem associated with the discrete spectrum $\sigma(H(\tau))$ is $\{E_j(\tau), |\Phi_j(\tau)\rangle\}_{j=0}^{M-1}$. Therefore the spectral theorem allows us to write:

$$H(\tau) = \sum_{j=0}^{M-1} E_j(\tau)|\Phi_j(\tau)\rangle\langle\Phi_j(\tau)|, \tag{6}$$

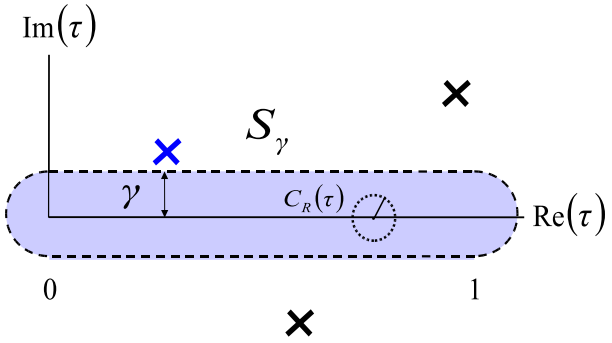

FIG. 1: Region of analyticity S_γ of the time-dependent, analytically continued Hamiltonian $H(\tau)$. The $\times$ symbols denote possible poles or branch points of $H(\tau)$.

[2] A "separable" vector space is one that admits a countable orthonormal basis.

[3] We assume analyticity in the sense of Kato [34][p.14]. Note that if $H(\tau)$ is a family of bounded operators, analyticity in the sense of Kato is equivalent to the definition of bounded operator-valued analytic functions.

where $\langle\Phi_i(\tau)|\Phi_j(\tau)\rangle = \delta_{ij}$, and $M = \dim(\mathcal{H}_n) = (\dim\mathcal{H})^n$. For notational convenience we will often write $|\Phi_0(\tau)\rangle \equiv |\Phi(\tau)\rangle$, and $E_0(\tau) \equiv E(\tau)$, though the "target" instantaneous eigenstate $|\Phi(\tau)\rangle$ need not necessarily be the ground state (see Fig. 2). The labeling in Eq. (6) is chosen such that it preserves ordering of the eigenvalues at the initial time (eigenvalues are continuous for all real τ, but not necessarily differentiable). This means that we allow the eigenvalues to cross [except with $E(\tau)$] (see Assumption 3).

Our second assumption further constrains the class of Hamiltonians:

Assumption 2 *It is possible to set any given number of the derivatives of the Hamiltonian $H(\tau)$ to zero at the initial and final times.*

This assumption is reasonable for "controllable" Hamiltonians of the type one envisions in AQC. We shall see that it will play a key role in constraining the error and in enforcing the right initial condition for AQC.

Our third assumption concerns the properties of the target state. Let

$$\mathrm{dist}(X, Y) \equiv \inf_{x\in X, y\in Y} |x - y|, \tag{7}$$

for any pair of sets $X, Y \subseteq \mathbb{C}$:

Assumption 3 *The "target" state $|\Phi(\tau)\rangle$, with the corresponding eigenvalue $E(\tau)$, is a nondegenerate and isolated eigenstate of $H(\tau)$.*

"Isolated" means that the spectrum $\sigma(H(\tau))$ has a gap structure around E — Fig. 2 — with a non-vanishing distance from the rest of the spectrum, i.e.:

$$\Delta_0(\tau) \equiv \mathrm{dist}\left(\{E(\tau)\}, \sigma(H(\tau))\backslash\{E(\tau)\}\right) > 0\ \forall\tau. \tag{8}$$

The minimum dimensionless spectral gap is

$$\Delta \equiv \inf_{\tau\in[0,1]} \Delta_0(\tau), \tag{9}$$

while in dimensional units we denote the minimum spectral gap by

$$d = J\Delta. \tag{10}$$

We shall often require the following quantity in our analysis:

$$\xi \equiv \sup_{\tau\in[0,1]} \left\|\frac{dh}{d\tau}\right\|, \tag{11}$$

where $\|\cdot\|$ denotes the standard operator norm defined in the next subsection. Note that ξ has units of energy. The projector onto the target subspace, and its complement, will also play important roles in our analysis:

$$P(\tau) \equiv |\Phi(\tau)\rangle\langle\Phi(\tau)|, \tag{12}$$

$$P_\perp(\tau) \equiv I - |\Phi(\tau)\rangle\langle\Phi(\tau)|. \tag{13}$$

In terms of these projectors, Eq. (6) can be replaced by the more general representation

$$H(\tau) = E(\tau)P(\tau) + P_\perp(\tau)H(\tau)P_\perp(\tau), \tag{14}$$

which does not depend on the existence of a discrete spectrum.

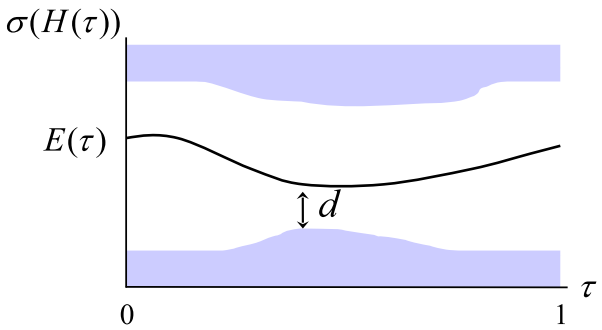

FIG. 2: Assumed gap structure in the spectrum of $h(\tau)$.

C. Norms and notation

We use the standard operator norm defined as the maximum singular value, which reduces for diagonalizable operators X to [24]:

$$\|X\| \equiv \sup_{\|v\|=1} |\langle v|X|v\rangle|, \tag{15}$$

where $X:\ \mathcal{V} \to \mathcal{V}$, $\mathcal{V} = \text{span}\{|m\rangle\}$ is a linear inner-product space with vectors $|v\rangle = \sum_m v_m|m\rangle$, for which

$$\|v\| \equiv \sqrt{\langle v|v\rangle} = \sqrt{\sum_m |v_m|^2} \tag{16}$$

is the standard Euclidean norm and $\langle m|m'\rangle = \delta_{mm'}$. We shall repeatedly use the submultiplicativity property of the operator norm [24]:

$$\|XY\| \leq \|X\|\|Y\|. \tag{17}$$

The minimum gap, the norm of the Hamiltonian and the rate at which the Hamiltonian changes, scale with the number n of subsystems. The parameter n is important for AQC because it represents the size of the computational problem. In the thermodynamic limit, systems with interesting computational properties undergo a quantum phase transition, i.e., the system will become gapless and the norms of the Hamiltonian will diverge. But for every finite n the system is finite and the gap can be assumed to be finite. Thus we introduce notation to make explicit that these quantities vary with n:

For all finite n the quantities $1/\Delta$, $\|\dot{H}\|$, and $\|\ddot{H}\|$ are finite:

$$1/\Delta \ \equiv \ A(n) < \infty, \tag{18}$$

$$\sup_{\tau\in[0,1]} \|\dot{H}\| \ \equiv \ \beta(n) = \xi(n)/J < \infty, \tag{19}$$

$$\sup_{\tau\in[0,1]} \|\ddot{H}\| \ \equiv \ \eta(n) < \infty, \tag{20}$$

where dot denotes $\partial/\partial\tau$. We can always take $A, \beta, \eta > 1$.

D. Adiabatic Theorem

We are now ready to state our main result. We wish to quantify the error in the adiabatic approximation, i.e., the distance between the actual final state $|\psi(T)\rangle$ and the target state $|\Phi(T)\rangle$ (both normalized). Since in quantum mechanics $|\psi(T)\rangle$ and $|\Phi(T)\rangle$ are rays in the projective Hilbert space $\mathcal{PH}_n$ [i.e., we identify $e^{i\zeta}|\psi(T)\rangle$ with $|\psi(T)\rangle$ and $e^{i\chi}|\Phi(T)\rangle$ with $|\Phi(T)\rangle$, where $\zeta, \chi \in \mathbb{R}$ are both arbitrary phases], the appropriate distance is $D = \arccos f$ (the Fubini-Study distance), where $f \equiv |\langle\psi(T)|\Phi(T)\rangle|$ is the "fidelity". As we shall see later [Eq. (48)], we shall obtain bounds for

$$\delta \equiv \||\psi(T)\rangle - e^{i\chi}|\Phi(T)\rangle\|, \tag{21}$$

where $\chi \in \mathbb{R}$ is a (dynamical) phase. Writing $\langle\psi(T)|\Phi(T)\rangle = \mathcal{F}e^{i\theta}$, where $0 \leq \{ \leq 1$ and $\theta \in \mathbb{R}$, we have $\delta = \sqrt{2[1 - \mathcal{F}\cos(\chi+\theta)]}$. Thus as long as $\cos(\chi+\theta) > 0$, an upper bound on δ is a lower bound on $\mathcal{F}$, and hence an upper bound on D. From now on we shall be concerned exclusively with the distance δ.

Theorem 1 *Given assumptions 1-3, and that the first $N+1$ derivatives of the Hamiltonian vanish at $\tau = 0$ and $\tau = 1$, a final time T which scales as*

$$T = \frac{q}{\gamma} N \frac{\xi(n)^2}{d(n)^3}, \tag{22}$$

where the "time dilation" $q > 1$ is a free parameter, yields an adiabatic approximation error which satisfies:

$$\delta \leq (N+1)^{\gamma+1} q^{-N}. \tag{23}$$

Thus, the adiabatic approximation error is exponentially small in the number N of vanishing H-derivatives, for a given time dilation q.

In several other papers, e.g., Refs. [9, 11], exponential error estimates in T that behave as $\delta \leq e^{-cT}$ have been proven, where c is some system-dependent constant. This applies in the setting where T is treated as an independent parameter and one considers a constant (time-dependent) Hamiltonian in a fixed Hilbert space. However, there are some important differences between our result and the works cited above. First, neither of Refs. [9, 11] extracted the time scale from the small parameter ϵ used in their expansions, which means that no direct physical interpretation of these results was given in terms of the adiabatic time. As we shall see, ϵ alone does not have a physical meaning. It is the combination of ϵ with the dimensional Hamiltonian and gap that will yield the time scale for the magnitude of the error. For the same reason, J drops out [see Eq. (112)]. Second, in Ref. [11] the error is not with respect to the instantaneous adiabatic eigenstate, but with respect to the superadiabatic basis, which has no immediate use for AQC. Let us now recast Theorem 1 in the form of an exponentially small error as a function of T, by eliminating N between Eqs. (22) and (23). In doing so we focus on the (simplified) exponential part (q^{-N}), since for $N \gg 1$ the polynomial factor $(N+1)^{\gamma+1}$ will be suppressed in comparison to the exponential factor. This gives an expression involving $q^{-1/q}$, which is minimized when $q = e$. We thus have (after re-inserting the polynomial factor):

Corollary 1 *Under the assumptions of Theorem 1 the adiabatic error satisfies*

$$\delta \lesssim (cT+1)^{\gamma+1}\, e^{-cT}, \tag{24}$$

where

$$c \equiv \frac{\gamma d^3}{e\xi^2}. \tag{25}$$

Thus our analysis reproduces the exponential error estimates obtained previously, but makes the dependence on the gap and rate of change of the Hamiltonian explicit.

Finally, in applications to AQC it may be sufficient to have a fixed error, as long as this corresponds to a success probability greater than $1/2$. It then follows from the Chernoff inequality [25] that one can then boost the confidence in the correct answer by repeating the adiabatic computation algorithm a few times.[4] By fixing an upper bound δ_u for the error, i.e., setting $\delta \leq \delta_u \equiv (N+1)^{\gamma+1} q^{-N}$, we can eliminate q and relate T directly to δ_u:

Corollary 2 *Under the assumptions of Theorem 1 a final time T which scales as*

$$T = (\delta_u)^{-\frac{1}{N}} \frac{1}{\gamma} N (N+1)^{\frac{\gamma+1}{N}} \frac{\xi(n)^2}{d(n)^3}, \tag{26}$$

yields an adiabatic error which satisfies:

$$\delta \leq \delta_u. \tag{27}$$

This corollary demonstrates that the adiabatic time T is insensitive to the adiabatic error (in that it depends only on its Nth root).

Remark 1 *The n-dependence of both ξ and the gap d is an important aspect of our result. It will be made explicit in Section VB. We also note again why we are interested in the N-dependence of T and δ. The reason is that we view N as a controllable parameter, which an experimenter or quantum algorithm designer can vary in order to optimize T and δ (see Section VB for more details).*

Remark 2 *The value of γ (distance of the nearest pole of the Hamiltonian in the complex time plane from the real time axis) may, in general, depend on the system size n. However, under certain natural assumptions for AQC which we specify in Section VB, γ is n-independent, so that the entire n-dependence of T comes from ξ and the gap d.*

Remark 3 *Because of our analyticity assumption, it is important that only a finite number N of derivatives of the Hamiltonian vanish at the initial and final times, for otherwise Liouville's theorem would imply that $H(\tau)$ would have to be constant (within its analyticity domain).*

Before proving Theorem 1 we briefly discuss resolvents and collect the pertinent results from Ref. [11] in Section III.

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[4] See Ref. [26] for an extensive discussion of related issues in quantum estimation algorithms.

III. BACKGROUND

A. Resolvents

Definition 2 *The (full) resolvent of H is:*

$$R(\tau, z) \equiv [H(\tau) - z]^{-1}. \tag{28}$$

It is defined on the resolvent set

$$\rho(H(\tau)) \equiv \mathbb{C} - \sigma(H(\tau)). \tag{29}$$

The resolvent is an analytic function of z on $\rho(H)$, and where $H(\tau)$ is an analytic function of τ, $R(\tau, z)$ will be an analytic function of τ as well [27]. By differentiating the identity $(H(\tau) - z)R(\tau, z) = I$, we obtain

$$\dot{R}(\tau, z) = -R(\tau, z)\dot{H}(\tau)R(\tau, z), \tag{30}$$

assuming that z and τ are independent.

Definition 3 *The reduced resolvent is a map from the full Hilbert space to the orthogonal complement of the target subspace:*

$$G_r(\tau) \equiv i[H(\tau) - E(\tau)]_r^{-1} : \mathcal{H}_n \to \mathcal{H}_n^{\perp} \equiv \mathcal{R}[P_{\perp}(\tau)], \tag{31}$$

(where $\mathcal{R}$ denotes the range) and is defined via

$$G_r(\tau)[H(\tau) - E(\tau)] = [H(\tau) - E(\tau)]G_r(\tau) = iP_{\perp}(\tau). \tag{32}$$

An explicit representation can be given in the case of a discrete spectrum [Eq. (6)]:

$$G_r(\tau) = \sum_{j>0} \frac{1}{\Delta_{j0}(\tau)} |\Phi_j(\tau)\rangle\langle\Phi_j(\tau)|, \tag{33}$$

where Δ_{j0} is the jth energy gap from the target state:

$$\Delta_{j0}(\tau) \equiv E_j(\tau) - E(\tau). \tag{34}$$

Also note that:

$$G_r(\tau)P_{\perp}(\tau) = P_{\perp}(\tau)G_r(\tau) = G_r(\tau). \tag{35}$$

B. Summary of main results from Ref. [11], and a modification

The main results we shall need from Ref. [11] are their Eqs. (2.10)–(2.19), which we reproduce here for convenience. First is the asymptotic expansion of an approximation to the full solution of the Schrödinger equation, where the zeroth order is the target adiabatic eigenstate:

$$|\Psi_N(\tau, \epsilon)\rangle \;=\; e^{-i\int_0^{\tau} E(\tau')d\tau'/\epsilon}(|\Phi(\tau)\rangle + \epsilon|\psi_1(\tau)\rangle + \epsilon^2|\psi_2(\tau)\rangle + \ldots + \epsilon^N|\psi_N(\tau)\rangle + \epsilon^{N+1}|\psi_{N+1}^{\perp}(\tau)\rangle). \tag{36}$$

The parameter ϵ is the one defined in Eq. (4). The vector $|\Psi_N(\tau, \epsilon)\rangle$ first appeared in Berry's work on the "superadiabatic approximation" [28], and is designed to provide a close approximation to the actual time-evolved state, under adiabatic evolution. We shall call $|\Psi_N(\tau, \epsilon)\rangle$ the "superadiabatic state", but it is important to note that it is not normalized, while $|\Phi(\tau)\rangle$ is. By inserting the superadiabatic state into the Schrödinger equation, and by choosing the phase of $|\Phi(\tau)\rangle$ so that

$$\langle\dot{\Phi}(\tau)|\Phi(\tau)\rangle = 0, \tag{37}$$

the following expressions have been obtained in Ref. [11]:

$$|\psi_j(\tau)\rangle \;=\; f_j(\tau)|\Phi(\tau)\rangle + |\psi_j^{\perp}(\tau)\rangle,\ 1 \le j \le N \tag{38}$$

$$|\psi_j^{\perp}(\tau)\rangle \;=\; G_r(\tau)\left(f_{j-1}(\tau)|\dot{\Phi}(\tau)\rangle + P_{\perp}(\tau)|\dot{\psi}_{j-1}^{\perp}(\tau)\rangle\right);\quad |\psi_0^{\perp}(\tau)\rangle \equiv 0, \tag{39}$$

where it follows from Eq. (35) that

$$\langle\Phi(\tau)|\psi_j^{\perp}(\tau)\rangle = 0,\ 1 \le j \le N+1, \tag{40}$$

explaining the "$\perp$" superscript.

The functions $f_j(\tau)$, $1 \le j \le N$, are determined by integration from their defining equation $\dot{f}_j = -\langle\Phi|\dot{\psi}_j^{\perp}\rangle$ [Eq. (2.11) in Ref. [11]] up to a constant c_j:

$$\begin{aligned} f_0(\tau) &\equiv 1, && (41)\\ f_j(\tau) &= -\int_0^{\tau} d\tau' \langle\Phi(\tau')|\partial_{\tau'}\psi_j^{\perp}(\tau')\rangle + c_j \\ &= \int_0^{\tau} d\tau' \langle\partial_{\tau'}\Phi(\tau')|\psi_j^{\perp}(\tau')\rangle + c_j, && (42) \end{aligned}$$

where the last equality follows from integration by parts and Eq. (40). In Ref. [11] the constants c_j were chosen to be zero, i.e., $f_j(0) = 0$, $1 \le j \le N$. For our purposes they are chosen so that

$$f_j(1) = 0, \quad 1 \le j \le N, \tag{43}$$

i.e., we choose $c_j = \int_0^1 d\tau' \langle\Phi(\tau')|\partial_{\tau'}\psi_j^{\perp}(\tau')\rangle$ for $1 \le j \le N$.

Equation (39) can also be written in either of the following forms:

$$\begin{aligned} |\psi_j^{\perp}\rangle &= G_r P_{\perp}\left(f_{j-1}|\dot{\Phi}\rangle + |\dot{\psi}_{j-1}^{\perp}\rangle\right) \\ &= G_r\left(f_{j-1}|\dot{\Phi}\rangle + |\dot{\psi}_{j-1}^{\perp}\rangle\right) \\ &= G_r|\dot{\psi}_{j-1}^{\perp}\rangle - f_{j-1}\dot{G}_r|\Phi\rangle. && (44) \end{aligned}$$

The first equality is to emphasize that G_r (and its derivatives) always come with a $P_{\perp}$ (although $P_{\perp}$ is already included in G_r). The last equality follows from Eq. (74) derived below.

Further, according to Eq. (2.19) in Ref. [11] we have:

$$\||\psi(\tau,\epsilon)\rangle - |\Psi_N(\tau,\epsilon)\rangle\| \le A_N(\tau)\epsilon^{N+1}, \tag{45}$$

where

$$A_N(\tau) \le \int_0^{\tau} \Big\|\frac{d\psi_{N+1}^{\perp}(\tau')}{d\tau'}\Big\| d\tau'. \tag{46}$$

The initial condition used in Ref. [11] is $|\psi(0,\epsilon)\rangle = |\Psi_N(0,\epsilon)\rangle$. Using Eqs. (36) and (38) we thus have $|\psi(0,\epsilon)\rangle = \sum_{j=0}^{N}\epsilon^j f_j(0)|\Phi(\tau)\rangle + \sum_{j=1}^{N+1}\epsilon^j|\psi_j^{\perp}(0)\rangle$. We shall show in Section IV B that we can make $|\psi_j^{\perp}(\tau_1)\rangle = 0$ for $1 \le j \le N+1$ by setting the first $N+1$ derivatives of H to zero at τ_1, and in particular at $\tau_1 = 0$. Thus we have

$$|\psi(0,\epsilon)\rangle = \vartheta|\Phi(\tau)\rangle, \quad \vartheta \equiv \sum_{j=0}^{N}\epsilon^j f_j(0), \tag{47}$$

and since $|\psi(0,\epsilon)\rangle$ and $|\Phi(\tau)\rangle$ are both normalized states, it follows that the initial state is the target state up to a pure phase factor $\vartheta \in \mathbb{C}$, namely $|\vartheta| = 1$.

IV. PROOF OF THEOREM 1

A. Proof strategy: two "adiabatic distances"

The central quantity of interest in the adiabatic theorem is the distance between the exact solution $|\psi(\tau,\epsilon)\rangle$ and the target eigenstate $|\Phi(\tau)\rangle$, at the final time. We define this "adiabatic distance" up to a phase (recall the discussion at the beginning of Section II D, where this phase was denoted by χ):

$$\delta \equiv \||\psi(1,\epsilon)\rangle - e^{-\frac{i}{\epsilon}\int_0^1 E(\tau')d\tau'}|\Phi(1)\rangle\|. \tag{48}$$

Using the triangle inequality we have

$$\delta \leq \delta_1 + \delta_2 \tag{49}$$
$$\delta_1 \equiv \| |\psi(1,\epsilon)\rangle - |\Psi_N(1,\epsilon)\rangle \| \tag{50}$$
$$\delta_2 \equiv \| e^{\frac{i}{\epsilon}\int_0^1 E(\tau')d\tau'} |\Psi_N(1,\epsilon)\rangle - |\Phi(1)\rangle \|. \tag{51}$$

Our strategy is to bound δ by considering δ_1 and δ_2 separately. We shall show that δ_1 can be bounded by a quantity that decreases exponentially in the asymptotic expansion order N. This will require the use of the analyticity of the Hamiltonian (Assumption 1). And, we shall show that δ_2 can be made to vanish by imposing that the first $N+1$ derivatives of the Hamiltonian vanish at the final time (Assumption 2). We start with δ_2 and the initial condition.

B. Role of boundary conditions on derivatives of the Hamiltonian

We now show that by introducing boundary conditions on the derivatives of H, we can impose that the initial $|\psi(0)\rangle$ is the eigenstate $|\Phi(0)\rangle$ up to a phase, and that $\delta_2 = 0$. The technique of imposing boundary conditions on the derivatives of H is inspired by the old work of Lennard [30] and Garrido and Sancho [31] (see also Nenciu's somewhat more recent work [32, 33]).

Lemma 1 *If $H^{(k)}(\tau_1) = 0$ for all $1 \leq k \leq N$ and for some $\tau_1 \in [0,1]$ then*

$$|\psi_j^{\perp}(\tau_1)\rangle = 0, \;\; j \in \{1,\ldots,N\}, \tag{52}$$

The proof is given in Appendix A. Using this Lemma we have:

Corollary 3 *If $H^{(k)}(0) = 0$ for all $1 \leq k \leq N+1$ then the initial condition is $|\psi(0,\epsilon)\rangle = \vartheta|\Phi(0)\rangle$, as in Eq. (47).*

Proof. Given above Eq. (47). ■

In AQC one envisions initializing the system in the ground state, which represents the input of the computational problem. Therefore, the last corollary confirms that we have the proper initial condition for AQC, since Assumption 3 guarantees that the target state is non-degenerate, and hence the global phase ϑ does not matter.

Moreover, we can make the error δ_2 vanish:

Corollary 4 *If $H^{(k)}(1) = 0$ for all $1 \leq k \leq N+1$ then $\delta_2 = 0$.*

Proof. It follows from Eqs. (36) and (38) that

$$\begin{aligned} e^{i\int_0^1 E(\tau')d\tau'/\epsilon}|\Psi_N(1,\epsilon)\rangle &= |\Phi(1)\rangle + \sum_{j=1}^{N}\epsilon^j|\psi_j(1)\rangle + \epsilon^{N+1}|\psi_{N+1}^{\perp}(1)\rangle \\ &= |\Phi(1)\rangle + \sum_{j=1}^{N}\epsilon^j f_j(1)|\Phi(1)\rangle + \sum_{j=1}^{N+1}\epsilon^j|\psi_j^{\perp}(1)\rangle \end{aligned} \tag{53}$$

Using Lemma 1 at $\tau_1 = 1$ and recalling that $f_0(\tau) = 1$ along with the boundary conditions $f_j(1) = 0$ for $j \geq 1$ [Eq. (43)] we thus have

$$e^{i\int_0^1 E(\tau')d\tau'/\epsilon}|\Psi_N(1,\epsilon)\rangle = |\Phi(1)\rangle, \tag{54}$$

from which it follows that $\delta_2 = 0$. ■

C. Operator and state bounds

In this section we derive bounds (many of which are not particularly tight) on the various operators and states that arise in the proof of Theorem 1.

From the definition (33) of the reduced resolvent and the definition of the operator norm as the maximum eigenvalue we immediately obtain

$$\|G_r(\tau)\| = \frac{1}{\text{dist}\left(\{E(\tau)\}, \sigma(H(\tau))\backslash\{E(\tau)\}\right)} \leq 1/\Delta = A(n). \tag{55}$$

Lemma 2

$$|\dot{\Phi}(\tau)\rangle = iG_r(\tau)\dot{H}(\tau)|\Phi(\tau)\rangle, \tag{56}$$

$$\dot{E}(\tau) = \langle\Phi(\tau)|\dot{H}(\tau)|\Phi(\tau)\rangle, \tag{57}$$

$$\ddot{E}(\tau) = \langle\dot{\Phi}(\tau)|\dot{H}(\tau)|\Phi(\tau)\rangle + \langle\Phi(\tau)|\dot{H}(\tau)|\dot{\Phi}(\tau)\rangle + \langle\Phi(\tau)|\ddot{H}(\tau)|\Phi(\tau)\rangle. \tag{58}$$

$$iP_\perp(\tau)|\ddot{\Phi}(\tau)\rangle = -G_r(\tau)\left(\ddot{H}(\tau) - \ddot{E}(\tau)\right)|\Phi(\tau)\rangle - 2G_r(\tau)\left(\dot{H}(\tau) - \dot{E}(\tau)\right)|\dot{\Phi}(\tau)\rangle, \tag{59}$$

Equation (57) is also known as the Hellmann-Feynman relation.

Proof. From Eq. (32), we have:

$$G_r(\tau)\dot{H}(\tau) = i\dot{P}_\perp(\tau) - \dot{G}_r(\tau)\left(H(\tau) - E(\tau)\right) + \dot{E}(\tau)G_r(\tau) \implies \tag{60}$$

$$\begin{aligned} G_r(\tau)\dot{H}(\tau)|\Phi(\tau)\rangle = & -i|\dot{\Phi}(\tau)\rangle\langle\Phi(\tau)|\Phi(\tau)\rangle - i|\Phi(\tau)\rangle\langle\dot{\Phi}(\tau)|\Phi(\tau)\rangle \\ & -\dot{G}_r(\tau)\left(H(\tau) - E(\tau)\right)|\Phi(\tau)\rangle + \dot{E}(\tau)G_r(\tau)|\Phi(\tau)\rangle. \end{aligned} \tag{61}$$

The second term on the RHS of Eq. (61) vanishes because of the phase condition (37) [11]; the third term vanishes because $H(\tau) - E(\tau)$ projects onto $\mathcal{H}_n^\perp$; the last term vanishes by Eq. (35). Thus using Eq. (33) we obtain the following formula for $|\dot{\Phi}(\tau)\rangle$:

$$|\dot{\Phi}(\tau)\rangle = iG_r(\tau)\dot{H}(\tau)|\Phi(\tau)\rangle \tag{62}$$

$$= \sum_{j\neq 0}\frac{\langle\Phi_j(\tau)|\dot{H}(\tau)|\Phi(\tau)\rangle}{\Delta_{j0}(\tau)}|\Phi_j(\tau)\rangle, \tag{63}$$

where the last equality holds for the case of a discrete spectrum, i.e., when Eq. (6) applies.

To obtain the Hellmann-Feynman relation (57), we differentiate the relations $E(\tau) = \langle\Phi(\tau)|H(\tau)|\Phi(\tau)\rangle$ and $\langle\Phi(\tau)|\Phi(\tau)\rangle = 1$. Another differentiation yields Eq. (58).

To obtain Eq. (59), we differentiate the eigenvalue equation $H|\Phi\rangle = E|\Phi\rangle$ twice. Thus:

$$(H - E)|\ddot{\Phi}\rangle = -(\ddot{H} - \ddot{E})|\Phi\rangle - 2(\dot{H} - \dot{E})|\dot{\Phi}\rangle. \tag{64}$$

Multiplying from the left by G_r and using Eq. (32), we obtain

$$iP_\perp|\ddot{\Phi}\rangle = -G_r(\ddot{H} - \ddot{E})|\Phi\rangle - 2G_r(\dot{H} - \dot{E})|\dot{\Phi}\rangle. \tag{65}$$

■

Corollary 5

$$\|\dot{\Phi}\| \leq A(n)\beta(n), \tag{66}$$

$$\|\dot{P}_\perp\| \leq 2A(n)\beta(n), \tag{67}$$

$$\|P_\perp|\ddot{\Phi}\rangle\| \leq 6A(n)^2\beta(n)^2 + 2A(n)\eta(n). \tag{68}$$

Proof. Equations (66) and (67) are immediate from Eqs. (19), (55), (56), and $\|\Phi(\tau)\| = 1$. From the Hellmann-Feynman relation, Eq. (57), and the definition of the operator norm, we have: $|\dot{E}(\tau)| \leq \|\dot{H}(\tau)\|$. Combining this with Eq. (58), we also obtain: $|\ddot{E}(\tau)| \leq 2\|\dot{H}(\tau)\|\|\dot{\Phi}(\tau)\| + \|\ddot{H}(\tau)\|$. Inserting these relations into Eq. (56), yields:

$$\|P_\perp|\ddot{\Phi}\rangle\| \leq \|G_r\|\left(\|\ddot{H}\| + \max|\ddot{E}| + 2(\|\dot{H}\| + \max|\dot{E}|)\|\dot{\Phi}\|\right). \tag{69}$$

Hence,

$$\|P_\perp|\ddot{\Phi}\rangle\| \leq \|G_r\|\left(2\|\ddot{H}\| + 6\|\dot{H}\|\|\dot{\Phi}\|\right) \leq 6A^2(n)\beta^2(n) + 2A(n)\eta(n). \tag{70}$$

■

Remark 4 *In Section V B we consider a general family of Hamiltonians relevant for AQC, for which we find that $\beta(n)$ and $\eta(n)$ have the same scaling with n [Eqs. (125) and (126)]. In this case we have the following bound, after we upper bound $2A(n)\eta(n)$ by $2A^2(n)\beta^2(n)$ (as is always possible for large enough n):*

$$\|P_\perp|\ddot{\Phi}\rangle\| \leq 8A^2(n)\beta^2(n). \tag{71}$$

Corollary 6

$$
\begin{aligned}
G_r(\tau)|\Phi(\tau)\rangle &= \langle\Phi(\tau)|G_r(\tau) = 0, && (72)\\
\langle\Phi(\tau)|\dot{G}_r(\tau) &= -\langle\dot{\Phi}(\tau)|G_r(\tau), && (73)\\
\dot{G}_r(\tau)|\Phi(\tau)\rangle &= -G_r(\tau)|\dot{\Phi}(\tau)\rangle, && (74)\\
\dot{G}_r(\tau)P_\perp(\tau) &= \dot{P}_\perp(\tau)G_r(\tau) + iG_r(\tau)[\dot{H}(\tau) - \dot{E}(\tau)]G_r(\tau), && (75)\\
\|\dot{G}_r(\tau)P_\perp(\tau)\| &\leq 4A^2(n)\beta(n). && (76)
\end{aligned}
$$

Proof. Equation (72) follows from Eq. (35). By differentiating Eq. (72) we immediately obtain Eqs. (73) and (74). From Eq. (32) we have

$$\dot{G}_r(\tau)[H(\tau) - E(\tau)] = i\dot{P}_\perp(\tau) - G_r(\tau)[\dot{H}(\tau) - \dot{E}(\tau)], \tag{77}$$

or after multiplying from the right by G_r and using Eq. (32) again:

$$\dot{G}_r(\tau)P_\perp(\tau) = \dot{P}_\perp(\tau)G_r(\tau) + iG_r(\tau)[\dot{H}(\tau) - \dot{E}(\tau)]G_r(\tau). \tag{78}$$

Bounding the norm of $\dot{G}_r P_\perp$ suffices for our analysis, for which Eqs. (55), (57), (66), and (78) yield:

$$\|\dot{G}_r(\tau)P_\perp(\tau)\| \leq 2A\beta \cdot A + A \cdot 2\beta \cdot A = 4A^2(n)\beta(n). \tag{79}$$

■

In the next lemma, and later in Eqs. (97) and (111), is where we use the assumption of analyticity of the Hamiltonian. This assumption is crucial for our error bound. The key technical tool is the Cauchy integral formula (which requires analyticity), which links the mth derivative of a function to its values in an explicit m-dependent way.

Lemma 3 *Let $B(0) = 1$ and $B(k) = k^k$, and let $D(k)$ and $\widetilde{D}(k)$ be arbitrary functions such that $\widetilde{D}(k) \geq D(k)\ \forall k \in \mathbb{N}$. Suppose $\varphi(\tau)$ is an analytic vector-valued function in the domain S_γ (Fig. 1). If $\varphi(\tau)$ satisfies*

$$\|\varphi(\tau)\| \leq D(k)B(k)(\gamma - |\mathrm{Im}(\tau)|)^{-k}, \tag{80}$$

for some $k \geq 0$, then $\dot{\varphi}(\tau) \equiv d\varphi(\tau)/d\tau$ satisfies

$$\|\dot{\varphi}(\tau)\| \leq \widetilde{D}(k)B(k+1)(\gamma - |\mathrm{Im}(\tau)|)^{-(k+1)}. \tag{81}$$

Proof. We reproduce and slightly generalize the proof reported in Ref. [11] (Lemma 3.1). This proof is more general than what is required in our case (Assumption 1), and we include it for completeness. Assume that $H(\tau)$ has poles or branch points at $\{\tau_i\}$, and let

$$\mu \equiv \min_i\{|\mathrm{Im}(\tau_i)|\}. \tag{82}$$

We consider a scenario wherein $H(\tau)$ can be analytically continued to the singularity-free open set (recall Fig. 1)

$$S_\mu \equiv \{\tau : |\tau| < \mu\} \cup \{\tau : |\mathrm{Im}(\tau)| < \mu, \mathrm{Re}(\tau) \in [0,1]\} \cup \{\tau : |\tau - 1| < \mu\}. \tag{83}$$

Define the circle $C_R(\tau) = \{\tau' \in S_\mu : |\tau - \tau'| = R(\tau) > 0\}$, centered at τ and with radius $R(\tau)$. This circle will shortly serve as an integration contour, and to ensure that $C_R(\tau)$ is always inside the set S_μ, it suffices to choose $\max_{\tau' \in C_R} |\mathrm{Im}(\tau')| = |\mathrm{Im}(\tau) + R(\tau)| < \mu$. Taking, for example, $R(\tau) = \frac{\mu - |\mathrm{Im}(\tau)|}{k+1}$, for some $k \geq 0$, satisfies this requirement. Relative to Assumption 1, where $\tau = 1$ and $\mu = \gamma$, all we require is $R < \gamma$.

The main idea is to use the Cauchy integral formula for the analytic function $\varphi(\tau)$ to write

$$\dot{\varphi}(\tau) = \frac{1}{2\pi i}\oint_{C_R(\tau)} \frac{\varphi(\tau')}{(\tau' - \tau)^2} d\tau',$$

where the circle $C_R(\tau)$ has radius $R(\tau) = \frac{\gamma - |\mathrm{Im}(\tau)|}{k+1}$. For $\tau' \in C_R(\tau)$, we have $|\mathrm{Im}(\tau')| \leq |\mathrm{Im}(\tau)| + R(\tau)$, hence $\gamma - |\mathrm{Im}(\tau')| \geq \frac{k}{k+1}(\gamma - |\mathrm{Im}(\tau)|)$. Replacing this bound in $\|\varphi(\tau)\| \leq D(k)B(k)(\gamma - |\mathrm{Im}(\tau)|)^{-k}$ [Eq. (80)], we obtain

$$\|\varphi(\tau')\| \leq D(k)\left(\frac{k}{(\gamma - |\mathrm{Im}(\tau')|)}\right)^k \leq D(k)\left(\frac{k}{\frac{k}{k+1}[\gamma - |\mathrm{Im}(\tau)|]}\right)^k. \tag{84}$$

Let $\widetilde{D}(k)$ be any function that upper-bounds $D(k)$ for all k. Then this gives rise to

$$\begin{aligned}\|\dot{\varphi}(\tau)\| &= \frac{1}{2\pi}\| \oint_{C_R(\tau)} \frac{\varphi(\tau')}{(\tau'-\tau)^2} d\tau' \| \\ &\leq \frac{1}{2\pi} \cdot 2\pi \frac{\gamma - |\mathrm{Im}(\tau)|}{k+1} \cdot \widetilde{D}(k) \cdot \left(\frac{k}{\frac{k}{k+1}[\gamma - |\mathrm{Im}(\tau)|]} \right)^k \cdot \left(\frac{1}{k+1}[\gamma - |\mathrm{Im}(\tau)|] \right)^{-2} \\ &= \widetilde{D}(k) \left(\frac{k+1}{\gamma - |\mathrm{Im}(\tau)|} \right)^{k+1}. \end{aligned} \tag{85}$$

The case $k = 0$ follows from the same argument by replacing $C_R(\tau)$ with $\alpha(\gamma - |\mathrm{Im}(\tau)|)$, for an arbitrary $\alpha < 1$. This results in the bound $\|\dot{\varphi}(\tau)\| \leq \widetilde{D}^{-1}(\gamma - |\mathrm{Im}(\tau)|)^{-1}$. In our application of Lemma 3 we use $D(k) = C(k)A^{a(k)}\beta^{b(k)}$ and $\widetilde{D}(k) = C(k)A^{c(k)}\beta^{d(k)}$, where $c(k) \geq a(k)$ and $d(k) \geq b(k)$, and where $C(k)$ is given in Eq. (106), $a(k)$ and $b(k)$ are the functions defined later in Eq. (103), $c(k)$ and $d(k)$ are the functions defined later in Eq. (104), and A and β are defined in Eqs. (18) and (19) (both are > 1), respectively. ■

D. Bound on δ_1

The error term δ_1 is exactly the one which already appeared in Eq. (46). Our strategy is to bound the integral in Eq. (46) by using an inductive approach based on Lemma 3. So far we have only used the differentiability property of $H(\tau)$, not its analyticity. If one wants to assume only that $H(\tau)$ is $N+1$-times differentiable, it is still possible to find an upper bound for the integral in Eq. (46), of course in terms of Δ as well as norms of derivatives of $H(\tau)$ — for an analysis based only on differentiability of the Hamiltonian, see, for example, Refs. [9, 12].

To apply Lemma 3, we first need to justify why $|\psi_{N+1}^{\perp}(\tau)\rangle$ is analytic in S_γ. We first show that by Assumption 1, $E(\tau)$ and $|\Phi(\tau)\rangle$ are analytic functions inside S_γ. To do so we recall the following theorem (modified slightly for our purpose here) [34]:

Theorem 2 (Kato-Rellich theorem) *Let $Q(\tau)$ be a family of bounded operator-valued analytic functions in a region S. Let $q(\tau_1)$ be a nondegenerate eigenvalue of $Q(\tau_1)$ — for our purpose, we take $\tau_1 \in \mathbb{R}$. Then, for τ near τ_1, there is exactly one point $q(\tau)$ of $\sigma(Q(\tau))$ near $q(\tau_1)$ and this point is isolated and nondegenerate. $q(\tau)$ is an analytic function of τ near τ_1, and there is an analytic eigenvector $|q(\tau)\rangle$. When $Q(\tau)$ is self-adjoint for $\tau - \tau_1 \in \mathbb{R}$, $|q(\tau)\rangle$ is also normalizable.*

Corollary 7 *$|\Phi(\tau)\rangle$ and $E(\tau)$ are analytic inside S_γ.*

Theorem 3 (XII.7 [34]) *Let $Q(\tau)$ be a family of bounded operator-valued analytic functions in a region S. Then the resolvent $R(\tau, z)$ of Q, for $z \in \rho(Q(\tau))$, is an analytic function of τ in S.*

Corollary 8 *$G_r(\tau)$ is an analytic function of τ inside S_γ.*

Proof. Let us take an arbitrary $z \in \rho(H(\tau))$. Then, by multiplying Eq. (32) by $R(\tau, z)$ from the right, we obtain

$$\begin{aligned} & G_r(\tau)\left[(H(\tau) - z) - (E(\tau) - z)\right] = iP_\perp(\tau) \implies \\ & G_r(\tau) = \frac{i}{z - E(\tau)} P_\perp(\tau) R(\tau, z) \left[P_\perp(\tau) R(\tau, z) - \frac{I}{E(\tau) - z} \right]^{-1}. \end{aligned}$$

Note that, since $\sigma(P_\perp(\tau)R(\tau,z)) = \{\frac{1}{E(\tau)-z};\ E(\tau) \in \sigma(H(\tau)) - \{E(\tau)\}, z \in \rho(H(\tau))\}$, the inverse on the RHS exists. Moreover, the expression on the RHS is analytic in terms of $R(\tau)$, which, together with analyticity of $P_\perp(\tau)$ in $\tau \in S_\gamma$, implies analyticity of $G_r(\tau)$ in S_γ. ■

Corollary 9 *$|\psi_{N+1}^{\perp}(\tau)\rangle$ is analytic inside S_γ.*

Proof. Note that $|\psi_1^{\perp}(\tau)\rangle = G_r(\tau)|\dot{\Phi}(\tau)\rangle$ is analytic, because of analyticity of $G_r(\tau)$ and $|\Phi(\tau)\rangle$ in S_γ, and because differentiation preserves analyticity. Now, let us assume by induction that $|\psi_j^{\perp}(\tau)\rangle$ is analytic. Analyticity of $|\psi_{j+1}^{\perp}(\tau)\rangle$ is then immediate from Eqs. (38) and (44):

$$|\psi_{j+1}^{\perp}(\tau)\rangle = G_r(\tau)\left[|\dot{\Phi}(\tau)\rangle \int_0^\tau d\tau' \langle \dot{\Phi}(\tau')|\psi_j^{\perp}(\tau)\rangle + |\dot{\psi}_j^{\perp}(\tau)\rangle \right], \quad 1 \leq j \leq N,$$

and the RHS is a product and sum of analytic functions. ■

Now we can initiate the application of Lemma 3. We assume that $\tau \in \mathbb{R}$ since we are only concerned with real time evolution in AQC. For notational simplicity we drop the τ-dependence from here on. From Eq. (44) we have:

$$|\psi_N^\perp\rangle = G_r P_\perp \left[f_{N-1}|\dot{\Phi}\rangle + |\dot{\psi}_{N-1}^\perp\rangle \right]. \tag{86}$$

We will find $\|\dot{\psi}_N^\perp\|$ by induction. To initialize the induction we use Eqs. (39) and (38):

$$|\psi_1^\perp\rangle = G_r P_\perp |\dot{\Phi}\rangle \overset{(55),(66)}{\Longrightarrow} \|\psi_1^\perp\| \leq A^2\beta, \tag{87}$$

$$\overset{(55),(66),(67),(68),(76)}{\Longrightarrow} |\dot{\psi}_1^\perp\rangle = \dot{G}_r P_\perp |\dot{\Phi}\rangle + G_r \dot{P}_\perp |\dot{\Phi}\rangle + G_r P_\perp |\ddot{\Phi}\rangle$$

$$\overset{(71),(79)}{\Longrightarrow} \|\dot{\psi}_1^\perp\| \leq 14A^3\beta^2. \tag{88}$$

We now assume by induction that

$$\|\psi_N^\perp\| \leq C(N) g(N) A^{a(N)} \beta^{b(N)}, \tag{89}$$

where $a(N)$, $b(N)$ and $C(N)$ are functions we shall determine, and where

$$g(N) = \left(\frac{N-1}{\gamma} \right)^{N-1} \qquad [g(1) \equiv 1]. \tag{90}$$

The form of $g(N)$ comes from Lemma 3. [5] Lemma 3 determines that differentiation raises $g(N)$ to $g(N+1)$. Setting $D(N) = C(N)A^{a(N)}\beta^{b(N)}$ and $\widetilde{D} = C(N)A^{c(N)}\beta^{d(N)}$ in that Lemma, provided $c(N) \geq a(N)$ and $d(N) \geq b(N)$, we obtain the bound:

$$\|\dot{\psi}_N^\perp\| \leq C(N) g(N+1) A^{c(N)} \beta^{d(N)}. \tag{91}$$

We shall determine $c(N)$ and $d(N)$ below.

Note that the initial conditions determined by Eqs. (87) and (88) are: [6]

$$a(1) = 2 \quad b(1) = 1, \tag{92}$$

$$c(1) = 3 \quad d(1) = 2, \tag{93}$$

$$C(1) = 1. \tag{94}$$

We now use the induction hypothesis to write

$$\|\psi_{N+1}^\perp\| \leq C(N+1) g(N+1) A^{a(N+1)} \beta^{b(N+1)}, \tag{95}$$

while on the other hand we have from Eq. (86)

$$\begin{aligned} \|\psi_{N+1}^\perp\| &= \|G_r \left[f_N |\dot{\Phi}\rangle + |\dot{\psi}_N^\perp\rangle \right]\| \\ &\leq \|G_r\| \left[|f_N| \|\dot{\Phi}\| + \|\dot{\psi}_N^\perp\| \right]. \end{aligned} \tag{96}$$

The inductive proof consists of showing that the bounds (95) and (96) are the same. To do so we first need to bound $|f_N|$:

$$\begin{aligned} |f_N(\tau)| &= \left| \int_0^\tau \langle \dot{\Phi}(\tau') | \psi_N^\perp(\tau') \rangle d\tau' \right| \\ &\leq \int_0^\tau \left| \langle \dot{\Phi}(\tau') | \psi_N^\perp(\tau') \rangle \right| d\tau' \\ &\leq \tau \cdot \sup_{\tau' \in [0,\tau]} \|\dot{\Phi}(\tau')\| \|\psi_N^\perp(\tau')\| \\ &\leq 1 \cdot A\beta \cdot C(N) g(N) A^{a(N)} \beta^{b(N)}, \end{aligned} \tag{97}$$

---

[5] Note that we have set $\mathrm{Im}(\tau) = 0$ because we are on the real axis.

[6] Note that the $g(2)$ factor present in Eq. (91) (evaluated at $N = 1$ and absent in Eq. (88)) gives rise to a discrepancy between the two bounds, unless we set $\gamma = 1/14$. This does in fact not impose a constraint on the family of Hamiltonians our proof applies to (recall Assumption 1), since in the application of Cauchy's theorem we are free to choose an arbitrarily small integration contour around the real-time axis. In spite of having thus fixed its value, we continue to write γ rather than $1/14$, as there is no fundamental importance to this value; it is merely an outcome of our rather loose bounds, e.g., as in Eq. (71).

where in the last step we used the induction hypothesis again, and hence also the analyticity assumption. Using this bound in (96) together with (91) we find:

$$\begin{aligned}\|\psi_{N+1}^{\perp}\| &\leq A\left[C(N)g(N)A^{a(N)+1}\beta^{b(N)+1}\cdot A\beta + 1\cdot C(N)g(N+1)A^{c(N)}\beta^{d(N)}\right]\\ &= C(N)\left[g(N)A^{a(N)+3}\beta^{b(N)+2} + g(N+1)A^{c(N)+1}\beta^{d(N)}\right]\\ &\leq C(N)\left[g(N)A^{a(N)+3}\beta^{b(N)+2} + g(N+1)A^{c(N)+1}\beta^{d(N)}(A\beta)^{k}\right]. \end{aligned} \tag{98}$$

In the last inequality we multiplied the second term by $(A\beta)^k$, where $k \geq 1$ is a constant, in order to allow for an adjustment to fit the initial conditions; see below. In order to complete the inductive proof the two bounds (95) and (98) should agree, and for this it is sufficient that their RHSs are equal:

$$C(N+1)g(N+1)A^{a(N+1)}\beta^{b(N+1)} = C(N)\left[g(N)A^{a(N)+3}\beta^{b(N)+2} + g(N+1)A^{c(N)+1+k}\beta^{d(N)+k}\right]. \tag{99}$$

Since A and β are arbitrary this requires that

$$C(N+1)g(N+1) = C(N)\left[g(N) + g(N+1)\right], \tag{100}$$

while the terms involving A and β must have equal powers, which implies:

$$a(N+1) = a(N) + 3 = c(N) + 1 + k, \tag{101}$$

$$b(N+1) = b(N) + 2 = d(N) + k. \tag{102}$$

From these last two equations, together with the initial conditions (92) we easily find:

$$a(N) = 3N - 1, \quad b(N) = 2N - 1. \tag{103}$$

We also have $c(N) = 3N + 1 - k$ and $d(N) = 2N + 1 - k$. The initial conditions (93) then yield $k = 1$, so that: [7]

$$c(N) = 3N, \quad d(N) = 2N. \tag{104}$$

Next we need to solve for $C(N)$ from Eq. (100), subject to the initial condition $C(1) = 14$. We have, using Eq. (90):

$$C(N+1) = C(N)\left(1 + \gamma\frac{(N-1)^{N-1}}{N^N}\right), \tag{105}$$

whose solution is

$$C(N) = \prod_{j=1}^{N-1}\left(1 + \gamma\frac{(j-1)^{j-1}}{j^j}\right). \tag{106}$$

We can upper-bound $C(N)$ as follows:

$$C(N) \leq \prod_{j=1}^{N-1}\left(1 + \gamma\frac{j^{j-1}}{j^j}\right) = \prod_{j=1}^{N-1}\frac{j+\gamma}{j} \leq \prod_{j=1}^{N-1}\frac{j+m}{j}, \tag{107}$$

---

[7] Another way to understand the need for the adjustment in the last line of Eq. (98) comes from this example:

$$\begin{aligned}\|\psi_2^{\perp}\| &\leq \|G_r\|\left[|f_1|\|\dot{\Phi}\| + \|P_{\perp}\|\|\dot{\psi}_1^{\perp}\|\right]\\ &\leq A^5\beta^3 + A^4\beta^2 \leq 2A^5\beta^3.\end{aligned}$$

To get the last inequality we multiplied the term $A^4\beta^2$ by $(A\beta)^k$ with $k = 1$. This is required in order to obtain a bound involving just a single power of A and of β. Failing to do this allows for the possibility that the two bounds (95) and (98) will not agree.

where $m = \lceil \gamma \rceil$ (smallest integer larger than γ). Thus

$$C(N) \leq \prod_{j=1}^{N-1} \frac{j+m}{j} = \frac{N(N+1)\cdots(N-1+m)}{m!} \tag{108}$$

$$\leq (N+1)(\frac{N}{2}+1)\cdots(\frac{N}{m}+1)$$

$$\leq (N+1)^m \leq (N+1)^{\gamma+1}. \tag{109}$$

By collecting all our results and inserting them into Eq. (91) we have, so far:

$$\|\dot{\psi}_N^{\perp}\| \leq (N+1)^{\gamma+1} \left(\frac{NA^3\beta^2}{\gamma}\right)^N. \tag{110}$$

From Eq. (46), we now have:

$$A_N(\tau) \leq \tau \cdot \sup_{0\leq s\leq\tau\leq 1} \|\dot{\psi}_{N+1}^{\perp}(s)\| \leq (N+2)^{\gamma+1} \left(\frac{(N+1)A^3\beta^2}{\gamma}\right)^{N+1}. \tag{111}$$

Reinserting dimensional units (i.e., $H = h/J$ and $\Delta = d/J$) we have

$$\delta_1 \equiv \||\psi(1,\epsilon)\rangle - |\Psi_N(1,\epsilon)\rangle\| \leq A_N(1)\epsilon^{N+1}$$

$$\leq (N+2)^{\gamma+1} \left(\frac{(N+1)(d/J)^{-3}(\sup_{\tau\in[0,1]} \|\dot{h}/J\|)^2}{\gamma}\right)^{N+1} (JT)^{-(N+1)}$$

$$= (N+2)^{\gamma+1} \left(\frac{(N+1)\xi^2}{\gamma T d^3}\right)^{N+1}, \tag{112}$$

where $\dot{h} \equiv \frac{dh}{d\tau}$.

Thus picking T as

$$T = \frac{q}{\gamma}(N+1)\frac{\xi^2}{d^3}, \tag{113}$$

where $q > 1$ is a "time dilation factor", gives:

$$\delta \leq (N+2)^{\gamma+1} q^{-(N+1)} \tag{114}$$

which can be made arbitrarily small in the number $N+1$ of zero derivatives of the Hamiltonian. We have thus proved Theorem 1 (where $N+1$ is redefined as N).

V. DISCUSSION

A. Comparison to the results of Jensen, Ruskai, and Seiler [12]

In Ref. [12], Jansen, Ruskai, and Seiler (JRS) proved — using the methodology of Avron *et al.* [10] rather than the asymptotic expansion [11] — a number of adiabatic theorems, all of which made weaker assumptions than ours. In particular, they did not assume analyticity. For example, their Theorem 3 can be summarized as follows. Assuming that $h(\tau)$ is C^2, that $\|\dot{h}\|$ and $\|\ddot{h}\|$ are both bounded, and that $\dot{h}(0) = \dot{h}(1) = 0$, then provided

$$T = q \int_0^1 \left(m\frac{\|\ddot{h}\|}{d_0^2} + 7m\sqrt{m}\frac{\|\dot{h}\|^2}{d_0^3}\right) d\tau, \tag{115}$$

the error at the final time can be made arbitrarily small in the "time dilation factor" $q > 1$:

$$\delta \leq q^{-2}. \tag{116}$$

Here $d_0(\tau) = J\Delta_0(\tau)$ is the instantaneous dimensional minimal gap [Eq. (8)], and the parameter $m(\tau)$ is the number of distinct eigenvalues in the spectrum of h restricted to the target subspace.

It is interesting to compare this result to our Theorem 1. In our case, by assumption the target subspace is one-dimensional, so $m \equiv 1$ (though this does not appear to be fundamental to our analysis). Furthermore, we have in various places replaced integrals over τ by the supremum of their integrand. In light of this, we would have written Eq. (115) as

$$T = 7q\frac{\xi^2}{d^3}, \tag{117}$$

which is indeed very similar to Eq. (22), except that the N-dependence is now absent. The reason for this is, of course, that JRS did not consider the case of N vanishing time derivatives. The fact that our error bound (23) is much tighter than JRS's (116) is again due to analyticity, which allowed us to introduce the N parameter into the error bound.

B. System-size dependent bounds for local Hamiltonians

Due to the appearance of $\sup_{\tau\in[0,1]} \|\frac{dh}{d\tau}\|^2$ in the expression for the adiabatic time (22), we now present norm bounds for physically relevant Hamiltonians, with the purpose of exhibiting the explicit system-size dependence to the extent possible. This is particularly relevant for AQC.

Let us consider the case when $h(\tau)$ is an L-local n-body Hamiltonian ($L \leq n$). An L-local Hamiltonian contains interaction terms involving at most L bodies, for some fixed L. For example, in the n-qubit case let $\{\boldsymbol{\sigma}\}$ be the operator basis constructed from tensor products of the Pauli matrices σ_x, σ_y, σ_z, and the identity matrix I. Then we can expand the Hamiltonian as:

$$H(\tau) = \sum_{\boldsymbol{\sigma}} \xi_{\boldsymbol{\sigma}}(\tau)\boldsymbol{\sigma}, \tag{118}$$

in which all $\xi_{\boldsymbol{\sigma}}$ are real functions. This expression for $H(\tau)$ is in fact a very general "interpolation" Hamiltonian, which captures many of the examples considered in the AQC literature, such as the common linear interpolation Hamiltonians of the type $H(\tau) = (1-\xi(\tau))H_0 + \xi(\tau)H_1$, where H_0 and H_1 are fixed, n-qubit Hamiltonians, and $\xi(0) = 0$, $\xi(1) = 1$ [5, 6, 20–22]. It also captures the unitary interpolation $H(\tau) = U(\tau)H(0)U^\dagger(\tau)$ [16], where $U(\tau)$ is unitary; this can be seen by Taylor expansion of $U(\tau)$.

For an L-local Hamiltonian, by definition $\xi_{\boldsymbol{\sigma}} = 0$ whenever the (Hamming) weight of the corresponding $\boldsymbol{\sigma}$ — the number of non-identity terms in the tensor product — is greater than L. The number of independent real parameters is [35]

$$\#(n, L) = \sum_{j=0}^{L} \binom{n}{j} 3^j \overset{L\leq n/2}{\leq} (L+1)\binom{n}{L}3^L. \tag{119}$$

In most physically relevant systems $L = 2$, i.e.,

$$H(\tau) = \sum_{j=1}^{n} V_j(\tau) + \sum_{j<j'} V_{jj'}(\tau). \tag{120}$$

In such cases, we have

$$\#(n, 2) = (9n^2 - 3n + 2)/2. \tag{121}$$

Putting together all these elements we find

$$\|H(\tau)\| \leq \#(n, 2) \cdot \sup_{\boldsymbol{\sigma}} |\xi_{\boldsymbol{\sigma}}(\tau)|. \tag{122}$$

Therefore, the overall upper bound for the scaling in terms of n is as follows:

$$\|H(\tau)\| = O\left(n^2 \cdot \sup_{\boldsymbol{\sigma}} |\xi_{\boldsymbol{\sigma}}(\tau)|\right) \leq O\left(n^2 \cdot \sup_{\boldsymbol{\sigma},\tau} |\xi_{\boldsymbol{\sigma}}(\tau)|\right). \tag{123}$$

With a similar analysis, we also obtain

$$\|H^{(k)}(\tau)\| \leq O\left(n^2 \cdot \sup_{\boldsymbol{\sigma},\tau} |\xi^{(k)}_{\boldsymbol{\sigma}}(\tau)|\right),\ k \in \mathbb{N}, \tag{124}$$

where $(\cdot)^{(k)} \equiv \frac{\partial^k}{\partial \tau^k}(\cdot)$. Usually, in physical systems of interest in condensed matter or quantum information, there is a predefined lattice or graph structure that dictates the spatial configuration of the system. Typically, there are n spins arranged on a 1D, 2D, or 3D lattice or graph. Increasing n in such systems means adding new particles only to the surface or boundary of the lattice. That is, by construction, a new particle cannot occupy a position inside the lattice, unless a structural defect is present. Even if there are structural defects in the system, it is plausible to assume that the number of defective sites is very small relative to the total number of the particles in the system, or this number may be a constant independent of n. Assuming that the interactions are only *local* (2-local in space and local in time) and *short-ranged*, therefore, new particles would not change the coupling strengths between the particles far enough from the surface. [8] This argument implies that in systems with a time-independent [9] and non-defective spatial graph/lattice structure, and short-ranged, local interactions, the coupling strengths (or interpolation functions) $\xi_{\boldsymbol{\sigma}}(\tau)$ do not depend on the system size n, for large enough n, and we have:

$$\|H(\tau)\| \leq \sup_{\boldsymbol{\sigma},\tau} |\xi_{\boldsymbol{\sigma}}(\tau)| \cdot O(n^2), \tag{125}$$

$$\|H^{(k)}(\tau)\| \leq \sup_{\boldsymbol{\sigma},\tau} |\xi^{(k)}_{\boldsymbol{\sigma}}(\tau)| \cdot O(n^2). \tag{126}$$

That is, the norm of $H(\tau)$ and all of its derivatives scale as $O(n^2)$, but with different coefficients.

A nice feature of the interpolation Hamiltonian (118) is that its analyticity is determined entirely by the scalar interpolation functions $\{\xi_{\boldsymbol{\sigma}}(\tau)\}_{\boldsymbol{\sigma}}$. Let $\gamma_{\boldsymbol{\sigma}}$ denote the height of the analyticity domain of $\xi_{\boldsymbol{\sigma}}(1)$. Then

$$\gamma = \inf_{\boldsymbol{\sigma}} \gamma_{\boldsymbol{\sigma}} \tag{127}$$

is the height of the analyticity domain appearing in Theorem 1. Clearly, if the interpolation functions $\xi_{\boldsymbol{\sigma}}(\tau)$ do not depend on the system size n because the system is confined to a graph with time-independent geometry and topology, nor will γ (recall Remark 2).

The next issue concerns the scaling of the gap with n. As pointed out, e.g., in Ref. [21], how the gap scales depends on whether one is dealing with a first or higher order quantum phase transition (QPT). First order QPTs are typically associated with exponentially small gaps, while higher order QPTs are associated with polynomially small gaps (in both cases, as a function of n). Consider first the latter, i.e.,

$$d(n) \sim Jn^{-z}, \tag{128}$$

where $z > 0$ is the "dynamical critical exponent" [36]. We can now apply these considerations to Theorem 1, and find:

Corollary 10 *Under the same assumptions as in Theorem 1, and assuming a second order quantum phase transition [i.e., a gap that scales as in Eq. (128)], a time scaling as*

$$T = \frac{q}{\gamma} N \frac{\left(\sup_{\boldsymbol{\sigma},\tau} |\dot{\xi}_{\boldsymbol{\sigma}}(\tau)|\right)^2}{J^3} n^{4-3z}, \tag{129}$$

yields an adiabatic approximation error which satisfies $\delta \leq (N+1)^{\gamma+1} q^{-N)}$ *(independently of* n*).*

A different situation arises in the context of the adiabatic version of Grover's problem [6], which is an example of a first order QPT. In Ref. [12], condition (115) was applied in this setting, where the Hamiltonian has the following form:

$$H_G(\tau) = (1 - x(\tau))(I - |\phi\rangle\langle\phi|) + x(\tau)(I - |m\rangle\langle m|), \tag{130}$$

(where $|\phi\rangle = \sum_{i=0}^{2^n-1} |i\rangle/\sqrt{2^n}$ and $m \in \{0, \ldots, 2^n - 1\}$) and the time-dependent spectral gap d_0 is found to have the following dependence on the number of qubits n:

$$d_0(n, \tau) = J\sqrt{2^{-n} + 4(1 - 2^{-n})(x(\tau) - 1/2)^2} \tag{131}$$

---

[8] Note that $\xi_{\boldsymbol{\sigma}}(\tau)$ may in general depend on n. One can see this through a simple example. Imagine a cylinder of gaseous particles with short-ranged interactions. Any particle will interact with all particles inside a sphere of radius r_{int} — the range of the interaction — around it. If we add new particles to the cylinder, at some point (i.e., at some n) all the space inside the shell will be occupied (close-packed), hence, the new particles cannot interact with the particle in the center. For such particles, the coupling strength of the interaction with the particle in the center is effectively zero.

[9] This condition is designed to exclude a folding of the system lattice, such as protein folding in the case of polymers or DNA molecules.

The minimum gap is encountered at the critical point, where the gap scales as $\Delta(n) = O(2^{-n/2})$. For this problem, condition (115) gives $T = O(d^{-1})$ for constant error. It is important in deriving this result that the function $x(\tau)$ is smooth (C^∞). This result is much more appealing in terms of its n-dependence than the general estimate (115), but it relies on the fact that the norm of the Hamiltonian does not scale with n: $\|H_G\| \leq 1 + 2\sup_\tau |x(\tau)|$, which is not the generic case. In the setting of our Theorem 1, it is clear that we would find $T = O(d^{-1})$ not for constant error, but for an error that can be made arbitrarily small. The assumption of a smooth Hamiltonian is of course compatible with our assumption of analyticity.

Recently, Ref. [23] derived another error estimate for AQC that relies on smooth interpolation and results in the same estimate for the running time: $T = O(d^{-1})$. To obtain this result Ref. [23] assumed again that the norm of the Hamiltonian is bounded above by a constant. Reference [23] also considered the case of a constant gap and highly degenerate first excited state (i.e., a Hamiltonian whose norm depends on n), and argued numerically that for a smooth interpolation it is possible to obtain an exponential error estimate: $\delta = O(n\exp(-Td))$, whence a running time $T = O(d^{-1}\ln n)$ suffices for arbitrarily small error. This case, though, is again non-generic. The generic situation is one in which the Hamiltonian couples all the states in the spectrum, and the spectral gap closes with n.

C. AQC related issues

In this subsection we collect a couple of observations related to the relevance of Theorem 1 to AQC.

First, as a general rule, an advantage in performing AQC over classical computation can only be guaranteed if one has *a priori* knowledge of the final time T, which is presumably shorter than the time required for the execution of the corresponding classical algorithm. Similarly, in our setting, in order to be able to set the final-time derivatives of the Hamiltonian equal to zero, one needs to know the final time T. Thus both in the general AQC setting and in our case one would like to know the gap d (as well as the other, more easily computable quantities appearing in Theorem 1). While this is sometimes amenable to an analytical solution, it is in almost all cases a very difficult problem. Fortunately, in AQC the gap is known exactly if one starts from a quantum algorithm given in the circuit model, by mapping this algorithm to the adiabatic model. In such a case the gap is an easily computable function of the number of gates [15, 37]. However, this result relies on a physically unreasonable Hamiltonian containing 5-body interactions, and recent results which map such Hamiltonians to physically reasonable 2-body interactions (e.g., Refs. [17, 18]), use so called "perturbative gadgets", which involve an approximation wherein the exact expression for the gap is lost. If one does not know the final time T exactly, one can still attempt to compute an estimate T_e for T, and set the final-time derivatives of the Hamiltonian equal to zero at T_e. Provided $T_e > T$, stretching the adiabatic evolution in such a manner cannot result in a worse error than promised by Theorem 1 for T.

Second, in the context of AQC one would like to measure the final state, in order to extract the answer to the computation. For this reason it makes sense to simply make the Hamiltonian constant for t starting from a value slightly smaller than T — which implies that the derivatives of the Hamiltonian at the final time T vanish. This, of course, automatically satisfies the requirement of vanishing final-time derivatives. One cannot make the same argument about initialization of the computation, however: initialization is a dynamic process (e.g., cooling into the ground state), so that one cannot keep the Hamiltonian constant for all $t < 0$.

D. The open system case

Suppose that our quantum system of interest S is coupled to another system B, which acts as an environment or "bath". This is the setting of open quantum systems [38]. Together, system and bath are described by the Hamiltonian

$$h(t) = h_S(t) \otimes I_B + h_{SB} + I_S \otimes h_B, \tag{132}$$

where h_S, h_{SB}, and h_B are the system, system-bath, and bath Hamiltonians, respectively, and I is the identity operator. The joint Hilbert space is $\mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_B$, where $\mathcal{H}_S$ and $\mathcal{H}_B$ are the system and bath Hilbert spaces. Then $h_{SB} : \mathcal{H} \mapsto \mathcal{H}$, $h_S : \mathcal{H}_S \mapsto \mathcal{H}_S$, and $h_B : \mathcal{H}_B \mapsto \mathcal{H}_B$. In our analysis above we only considered $h_S(t)$, which implements the adiabatic system evolution in the present case. We assume that h_{SB} and h_B are time-independent Hamiltonians. This is a reasonable physical assumption in many cases [38].

Coupling of the system to the bath introduces decoherence, and modifies the adiabatic condition relative to the closed system case we have discussed thus far [39–42]. We are interested in the adiabatic theorem which describes the system state alone. To this end, we need an appropriate distance measure. The trace distance is defined as $D[\rho_1, \rho_2] \equiv \frac{1}{2}\|\rho_1 - \rho_2\|_1$, where $\|A\|_1 \equiv \mathrm{Tr}|A|$, $|A| \equiv \sqrt{A^\dagger A}$, and is a good distance measure between states (or density matrices) ρ_1 and ρ_2 acting on the same Hilbert space [14]. A useful fact is that taking the partial trace can only decrease the distance between states [14], i.e., if ρ_1 and ρ_2 are states in the joint system-bath Hilbert space $\mathcal{H}$, then

$$D[\mathrm{Tr}_B\rho_1, \mathrm{Tr}_B\rho_2] \leq D[\rho_1, \rho_2], \tag{133}$$

where Tr_B is the partial trace operation over the bath Hilbert space: $\mathrm{Tr}_B[|s\rangle\langle s'| \otimes |b\rangle\langle b'|] \equiv \langle b'|b\rangle|s\rangle\langle s'|$, for arbitrary states $|s\rangle, |s'\rangle \in \mathcal{H}_S$ and $|b\rangle, |b'\rangle \in \mathcal{H}_B$. Inequality (133) can be understood intuitively as a consequence of the fact that by erasing information (taking the partial trace) one cannot make states more distinguishable, i.e., their distance cannot increase.

Consider first the *uncoupled* setting $h_{SB} = 0$, which we denote by the superscript 0. The target adiabatic system state is $\rho^0_{S,\mathrm{ad}}(t) = |\Phi(t)\rangle\langle\Phi(t)|$. Let $\rho^0_{\mathrm{ad}}(t) \equiv \rho^0_{S,\mathrm{ad}}(t) \otimes \rho^0_B(t)$ denote the "target adiabatic joint state," with $\rho^0_B(t) = e^{-ih_B t}\rho^0_B(0)e^{ih_B t}$. Let $\rho(0)$ denote the initial joint system-bath state. The *actual* state whose time evolution is generated by $h(t)$ [Eq. (132)] is $\rho(t) = U(t)\rho(0)U(t)^\dagger$, where $U(t) = \mathcal{T}e^{-i\int_0^t h(t')dt'}$ is the propagator of the joint system-bath dynamics, with $\mathcal{T}$ denoting time ordering. The actual time evolved system state is $\rho_S(t) = \mathrm{Tr}_B\rho(t)$. Using Eq. (133), we have the following inequality:

$$\delta_S \equiv D[\rho_S(T), \rho^0_{S,\mathrm{ad}}(T)] \leq D[\rho(T), \rho^0_{\mathrm{ad}}(T)] \equiv \delta_{SB}. \tag{134}$$

The distance δ_S is the distance of interest: it is the distance between the actual system state and target system adiabatic state. The last inequality shows that it is upper-bounded by the distance δ_{SB} between two "closed-system" states, where closed refers here to the joint system-bath entity. Because of this, we already know the form of the adiabatic theorem for δ_{SB}. This is just Theorem 1 again, with h as prescribed in Eq. (132). It follows from Eq. (134) that we can use this upper bound on δ_{SB} to bound δ_S as well. To be explicit, let us state the theorem we thus obtain for the open system case:

Theorem 4 *Let d denote the minimum gap of the full Hamiltonian $h(t)$ in Eq. (132). Given assumptions 1-3 on $h(t)$, assuming h_B and h_{SB} are time-independent, and that the first $N+1$ derivatives of the Hamiltonian vanish at $\tau = 0$ and $\tau = 1$,a final time T which scales as*

$$T = \frac{q}{\gamma}N\frac{\sup_{\tau\in[0,1]}\|\dot{h}_S\|^2}{d^3}, \tag{135}$$

where $q > 1$ is a free parameter, yields an adiabatic approximation error which satisfies:

$$\delta_S \leq \delta_{SB} \leq (N+1)^{\gamma+1}q^{-N} \tag{136}$$

Remark 5 *There is an important difference between the closed and open system cases: the minimum gap d in the open system case is the gap for the full system-bath Hamiltonian (132), which can be expected to be significantly smaller than for the isolated system, since generally, due to its much larger number of degrees of freedom, the bath will introduce many intermediate levels inside the gap depicted in Fig. 2 for the isolated system. This means that T can be expected to be very much larger in the open system case than for the same system without coupling to a bath. See also Ref. [39] for a different approach leading to the same conclusion.*

VI. CONCLUSIONS

In this work we aimed to bridge a gap between rigorous formulations of the quantum adiabatic theorem, leading to exponentially tight error estimates, and the field of adiabatic quantum computation (AQC), where knowledge of the way the energy gap enters the conditions for the adiabatic approximation is crucial. To this end we have presented a version of the quantum adiabatic approximation that is useful for AQC, where there is a single non-degenerate ground state, the number of subsystems n is variable, and where the interpolation from the initial to the final Hamiltonian is fully controllable, at least in principle. In this case, we have shown that for a total time T scaling as the product of the cube of the inverse gap and the square of the operator norm of $\dot{h}$, the error in the adiabatic approximation can be made exponentially small. Since our version of the quantum adiabatic theorem explicitly accounts for the system size dependence (see, e.g., Corollary 10), this represents an advance over previous adiabatic theorems, where either the approximation error or the system-size dependence is not nailed down.

Our results imply that as long as our key assumption of analyticity of the interpolation in a domain can be satisfied, along with a degree of control that allows setting the initial and final time derivatives of the Hamiltonian equal to zero, then from a closed-system perspective AQC has an important fault tolerance advantage over the circuit model of quantum computation [14]. Namely, whereas in the circuit model even unitary deviations from a prescribed set of gates can ruin a quantum algorithm, in AQC large deviations are permissible, as long as the interpolation ends at the desired final Hamiltonian, whose ground state encodes the answer to the computational problem one is trying to solve. Of course, this should not be misinterpreted as a claim that AQC is fully fault tolerant. It is well known that AQC is vulnerable to interactions with the environment [40, 44–48], and only preliminary steps have been taken towards a theory of fault tolerant AQC in an open systems setting [43, 49]. We have also reported a corollary regarding the adiabatic theorem for open quantum systems (Theorem 4), which shows that the time-scale for adiabaticity is determined by the gap of the full system-bath Hamiltonian.

There are indications that the adiabatic approximation fails for Hamiltonians with several independent time-scales [50] (see also Ref. [12]). This presents an interesting problem for AQC, even in our setting of a closed system with analytic Hamiltonians.

For example, consider a situation where there is some smooth control noise on the interpolation functions $\xi_{\boldsymbol{\sigma}}(\tau)$, which has an independent time-scale. Then merely slowing down the evolution by elongating T will have no impact on this noise, so that in its presence the time dilation-based error bound (23) cannot be expected to apply. In other words, noise with an intrinsic time scale that cannot be stretched in the sense that makes ϵ in the asymptotic expansion (36) small, generates a violation of the assumptions used to derive the adiabatic theorem. Future work on fault-tolerant AQC should address this problem.

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APPENDIX A: PROOF OF LEMMA 1

We first need the following Lemma:

Lemma 4 *If $H^{(k)}(\tau_1) = 0$ for all $1 \leq k \leq N$ and for some $\tau_1 \in [0,1]$, then*

$$E^{(k)}(\tau_1) = P^{(k)}(\tau_1) = |\Phi^{(k)}(\tau_1)\rangle = 0,\ k \in \{1,\ldots,N\}. \tag{A1}$$

Proof. It is well known that for a closed operator $H(\tau)$ with $E(\tau)$ an isolated point of $\sigma(H(\tau))$ (i.e., suppose that for some ε: $\sigma(H) \cup \{E' :\ |E - E'| < \varepsilon\} = \{E\}$), the corresponding projection can be written as

$$P(\tau) = \frac{1}{2\pi i} \oint_{|E-E'|=r} dE' R(\tau, E'), \tag{A2}$$

for any $r \in (0, \varepsilon)$ [34], where $R(\tau, E')$ is the full resolvent of $H(\tau)$. Since $E(\tau)$ is the eigenvalue of $H(\tau)$ associated with the eigenstate $|\Phi(\tau)\rangle$ we have:

$$E(\tau) = \mathrm{Tr}[H(\tau)P(\tau)]. \tag{A3}$$

By differentiating Eqs. (A2) and (A3) and using Eq. (30), we obtain

$$\dot{P}(\tau) \ = \ -\frac{1}{2\pi i} \oint_{|E-E'|=r} dE' R(\tau, E') \dot{H}(\tau) R(\tau, E'), \tag{A4}$$

$$\dot{E}(\tau) \ = \ \mathrm{Tr}[\dot{H}(\tau)P(\tau)] + \mathrm{Tr}[H(\tau)\dot{P}(\tau)]. \tag{A5}$$

Thus making $\dot{H}(\tau_1) = 0$ implies $\dot{P}(\tau_1) = 0$, which in turn, from Eq. (A5), implies $\dot{E}(\tau_1) = 0$ as well. Note that $\dot{P}(\tau_1) = 0$ also implies $\dot{P}_\perp(\tau_1) = 0$. Moreover, Eq. (56) yields:

$$|\dot{\Phi}(\tau_1)\rangle = iG_r(\tau_1)\dot{H}(\tau_1)|\Phi(\tau_1)\rangle = 0. \tag{A6}$$

By simple applications of the Leibniz rule ($(X \cdot Y)^{(k)} = \sum_{i=0}^{k} \binom{k}{i} X^{(i)} \cdot Y^{(k-i)}$, for any pair of (differentiable) objects), it can be seen that these conclusions hold also for higher order derivatives. We show this explicitly for $|\Phi^{(k)}(\tau_1)\rangle$. We obtain

$$|\Phi^{(k)}(\tau_1)\rangle = i \sum_{i=0}^{k-1} \binom{k}{i} G_r^{(i)}(\tau_1) \left(\dot{H}|\Phi\rangle\right)^{(k-i)} |_{\tau_1}. \tag{A7}$$

All terms within the summation include a derivative of H. The highest derivative in the RHS is $H^{(k)}$. This is zero for all $k \leq N$. That is, $|\Phi^{(k)}(\tau_1)\rangle = 0,\ k \in \{1,\ldots,N\}$. ■

Corollary 11 *Under the assumptions of Lemma 4, we have*

$$H^{(k)}(\tau_1) = 0 \Longrightarrow G_r^{(k)}(\tau_1) = 0,\ k \in \{1, \ldots, N\}. \tag{A8}$$

Proof. Using Eqs. (74) and the definition of $P_\perp$ we have $\dot{G}_r P_\perp = \dot{G}_r + G_r|\dot{\Phi}\rangle\langle\Phi|$. Thus, using Eqs. (75) and Lemma 4 we find:

$$\dot{G}_r(\tau_1) = -G_r(\tau_1)|\dot{\Phi}(\tau_1)\rangle\langle\Phi(\tau_1)| + \dot{P}_\perp(\tau_1)G_r(\tau_1) + iG_r(\tau_1)[\dot{H}(\tau_1) - \dot{E}(\tau_1)]G_r(\tau_1) = 0.$$

From the Leibniz rule we obtain

$$\begin{aligned} G_r^{(k)}(\tau_1) \ &= \ -\sum_{i=0}^{k-1} \binom{k-1}{i} G_r^{(i)}(\tau_1) \left(|\dot{\Phi}\rangle\langle\Phi|\right)^{(k-1-i)}|_{\tau_1} \\ &\quad + \sum_{i=0}^{k-1} \binom{k-1}{i} P_\perp^{(i+1)}(\tau_1) G_r^{(k-1-i)}(\tau_1) \\ &\quad + i\sum_{i=0}^{k-1} \binom{k-1}{i} G_r^{(i)}(\tau_1) \left([\dot{H} - \dot{E}]G_r\right)^{(k-1-i)}|_{\tau_1}. \end{aligned} \tag{A9}$$

From Lemma 4, all the terms within the summations vanish for all $k \leq N$. ■

We are now ready to give the proof of Lemma 1.

of Lemma 1. We note that $|\psi_1^\perp(\tau)\rangle = G_r(\tau)|\dot{\Phi}(\tau)\rangle \overset{(74)}{=} -\dot{G}_r(\tau)|\Phi(\tau)\rangle$, from which by using Corollary 11 we obtain

$$|\psi_1^\perp(\tau_1)\rangle = \ -\dot{G}_r(\tau_1)|\Phi(\tau_1)\rangle = 0, \tag{A10}$$

$$|\dot{\psi}_1^\perp(\tau_1)\rangle = \ -\ddot{G}_r(\tau_1)|\Phi(\tau_1)\rangle - \dot{G}_r(\tau_1)|\dot{\Phi}(\tau_1)\rangle = 0, \tag{A11}$$

or in general, using the Leibniz rule:

$$\partial_\tau^k|\psi_1^\perp(\tau_1)\rangle = -\sum_{i=0}^{k} \binom{k}{i} G_r^{(i+1)}(\tau_1)|\Phi^{(k-i)}(\tau_1)\rangle = 0\ , 0 \leq k \leq N-1, \tag{A12}$$

since each term inside the summation vanishes as long as $G_r^{(i+1)}(1) = 0$, i.e., $i+1 \leq N$, or, $k = N-1$.

We now show by induction that if $\partial_\tau^k|\psi_{j-1}^\perp(\tau_1)\rangle = 0$ for $0 \leq k \leq N-(j-1)$, then $\partial_\tau^k|\psi_j^\perp(\tau_1)\rangle = 0$ for $0 \leq k \leq N-j$. The calculation above initialized the induction for $j = 2$. We have by Eq. (44):

$$\begin{aligned} \partial_\tau^k|\psi_j^\perp(\tau_1)\rangle \ &= \ -f_{j-1}(\tau_1)\left(\dot{G}_r|\Phi\rangle\right)^{(k)} - \sum_{i=1}^{k} \binom{k}{i} f_{j-1}^{(i)}(\tau_1)\left(\dot{G}_r|\Phi\rangle\right)^{(k-i)} \\ &\quad + \sum_{i=1}^{k} \binom{k}{i} G_r^{(i)}(\tau_1)|\psi_{j-1}^{(k-i+1)}(\tau_1)\rangle + G_r(\tau_1)|\psi_{j-1}^{(k+1)}(\tau_1)\rangle. \end{aligned} \tag{A13}$$

As long as $k \leq N$ all the terms within the summations are zero, because each of them contains a derivative of G_r at most up to order N. The first term generates a $G_r^{(k+1)}(\tau_1)$. When $k+1 \leq N$, this term also vanishes. By assumption, the last term vanishes when $k+1 \leq N-(j-1)$. Since $j \geq 2$ this implies that all terms vanish when $k \leq N-j$. Overall, we have shown that

$$\partial_\tau^k|\psi_j^\perp(\tau_1)\rangle = 0,\ \text{for}\ 1 \leq j \leq N,\ 0 \leq k \leq N-j. \tag{A14}$$

Immediate corollaries of this result are as follows:

$$|\psi_j^\perp(\tau_1)\rangle \quad = \quad 0,\ 1 \leq j \leq N, \tag{A15}$$

$$|\psi_j(\tau_1)\rangle \quad \overset{(38)}{=} \quad f_j(\tau_1)|\Phi(\tau_1)\rangle,\ 1 \leq j \leq N, \tag{A16}$$

$$\partial_\tau^k f_j(\tau_1) \quad \overset{(38),(A14)}{=} \quad 0,\ 1 \leq j \leq N,\ 1 \leq k \leq N-j. \tag{A17}$$

This concludes the proof. ■

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